MM 35: Methods in Computational Materials Modelling IV: Steels

Time: Wednesday 11:45–13:15 Location: H 0106

MM 35.1 Wed 11:45 H 0106

Temperature-dependent magnon-phonon coupling in bcc Fe — •Fritz Körmann, Blazej Grabowski, Biswanath Dutta, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

An ab initio based framework for quantitatively assessing the non-adiabatic free energy contributions due to magnon-phonon interactions and lattice expansion to phonon energies is developed [1]. Employing the framework of the recently developed spin-space averaging (SSA) procedure provides paramagnetic forces at high temperatures [2]. The full temperature dependence of phonons for arbitrary magnetic temperatures is obtained by relating the ferromagnetic and paramagnetic SSA force constants with energetics from the magnetic subsystem. The latter is derived by means of QMC simulations for an effective Heisenberg model [3]. The theoretical results for bcc Fe are in very good agreement with recent high-quality phonon frequency measurements [1]. For some phonon branches, the impact of magnetic excitations is an order of magnitude larger than the phonon shift due to lattice expansion. The significant role of magnetic short-range order on lattice vibrations above the Curie temperature is demonstrated.

[1] F. Körmann, B. Grabowski, B. Dutta, T. Hickel, L. Mauger, B. Fultz, J. Neugebauer, Phys. Rev. Lett. 113, 165503 (2014).

[2] F. Körmann, A. Dick, B. Grabowski, T. Hickel, J. Neugebauer, Phys. Rev. B 85, 125104 (2012).

[3] F. Körmann, A. Dick, T. Hickel, and J. Neugebauer, Phys. Rev. B 83, 165114 (2011).

MM 35.2 Wed 12:00 H 0106

Characterisation of transformations at disordered FeCr bcc-σ interfaces — •Thomas Schablitzki, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Deutschland

Using an adaptive kinetic Monte Carlo (akMC) approach, we study the transformation of the σ-phase in FeCr to the bcc structure. During the transformation we observe disordered interface regions with a thickness of several atomic layers. Transformation paths from one crystal phase to another become obfuscated by seemingly random movements and rearrangements at the interface. This creates a challenge in studying the atomistic processes that drive the transformation.Based on our akMC trajectories we analyse the topology of the potential energy surface and the influence of excessive loops on the transformation paths. Using coordination polyhedra and topological fingerprints we look for correlations in processes in the interface region of FeCr bcc-σ interfaces and along the transformation paths trying to identify characteristic processes of the phase transition.

MM 35.3 Wed 12:15 H 0106

Multi-scale description of super-saturated ferrite in severely deformed pearlitic wires — •Nematollahi Gh. Ali, Grabowski Blazej, Raabe Dierk, and Neugebauer Jörg — Max-Planck Institut für Eisenforschung, D-40237 Düsseldorf, Germany

Severely deformed pearlitic wires are the strongest structural materials with up to 7 GPa strength. Despite extensive research the fundamental mechanisms underlying the extraordinary strength are unclear. Experimental evidence suggests a substantial cementite decomposition resulting in a dramatically increased C concentration in the ferrite matrix which is 9 orders of magnitude above phase diagram predictions. To study the stability of C interstitials in ferrite and of C vacancies in cementite in the presence of elastic strain and dislocations we have developed a multi-scale approach using density functional theory, embedded atom potentials and an empirical model. A careful analysis reveals that a strain-induced stabilization of the C interstitial in ferrite in conjunction with a stabilization of the C trapping sides around dislocations enhance the carbon solubility strongly. Based on this insight we are able to explain the experimentally observed super-saturation of ferrite and the partial dissolution of cementite in severely deformed pearlite.

MM 35.4 Wed 12:30 H 0106

Z phase strengthened steels for ultra-supercritical power plants — •Daniel F. Urban, Christian Elsässer, and Hermann Riedel — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

To minimize fuel consumption and CO2 emission of fossil fired power plants, the thermal efficiency, and therefore the steam inlet temperatures, must be as high as possible. In the past 30 years sufficiently creep resistant 9% chromium steels were developed, allowing steam temperatures up to 615 °C. The increased creep resistance was obtained by controlled precipitation of fine (V,Nb)N particles. Further raise of the steam temperature calls for higher Cr contents for better corrosion and oxidation resistance. However, 11-12% Cr ferritic-martensitic steels strengthened by fine (V,Nb)N particles reveal that precipitation of the thermodynamically stable Z-phase, Cr(V,Nb,Ta)N, in long-term service is unavoidable and detrimental. Usually, coarse and brittle Z-phase particles grow at the expense of the desired fine nitride particles. We follow the idea to exploit the Z-phase as strengthening agent in martensitic creep resistant 12% Cr steels by controlling the precipitation of the Z-phase such that fine, thermodynamically stable Z particles are formed. We present atomistic DFT simulations which reveal the essential mechanisms underlying the Z-phase formation. Chromium atoms diffuse into nitride particles and subsequently cluster in a layered arrangement which finally yields the transformation of the nitride particles to Z-phase.

MM 35.5 Wed 12:45 H 0106

Calculation of Electronic Thermophysical Parameters for Steel Alloys based on Density Functional Theory — •Juergen Sotrop[1], Jan Winter[1], Heinz P. Huber[1], Stephan Borek[2], and Jan Minar[2,3] — [1]Munich University of Applied Sciences — [2]Ludwig-Maximilians Universit, Muenchen — [3]University of West Bohemia, Pilsen

The ablation mechanism of matter irradiated with ultra-short laser pulses has been widely investigated over the last two decades. At present there is still lack of theoretical understanding of the interaction of ultra-short laser pulses with a metal alloy. By irradiating material with ultra-short laser pulses initially strong electron-phonon nonequilibrium will occur. The resulting difference in electron and phonon temperatures can be calculated with the so called two-temperature model (TTM). An essential prerequisite for the application of the TTM is a determination of the temperature dependent thermophysical parameters such as electron heat capacity and electron-phonon coupling factor. We will present a general method for the calculation of the electronic thermophysical parameters for metal alloys, here performed exemplarily on stainless steel (AISI 304). The method is based on the calculation of the electronic density of states (DOS) using a fully relativistic implementation of the KKR-formalism in the framework of spin density functional theory. Precise knowledge of the DOS will enable the calculation of the electron-phonon-coupling factor and the electron heat capacity. The model is compared with the well-known parameters for iron to show the validity.

MM 35.6 Wed 13:00 H 0106

New metastable phases of the Cr_xSb_y system with different $x:y$ ratios: theory and experiment — •Svitlana Polesya[1], Gerhard Kuhn[1], Sergiy Mankovsky[1], Matthias Regus[2], Wolfgang Bensch[2], and Hubert Ebert[1] — [1]Dept. Chemie/Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Deutschland — [2]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, Max-Eyth-Str. 2, D-24118 Kiel, Deutschland

The present investigation aims to find new metastable phases of the Cr-Sb system as well as of some other compounds based on it. Corresponding experimental investigations are supported by theoretical first principle calculations which allow to predict the physical properties of new compounds and alloys and to explain the behaviour of new phases synthesized experimentally. In particular we focus on the Cr_xSb_y compounds with the ratios $x:y = 2:1, 1:2$, and $1:3$. In the case of the non-stoichiometric $Cr_{1+x}Sb$ compound a new Cr-rich phase has been obtained which crystallizes in the Ni_2In-like structure. The structure parameters for this system obtained via ab-initio total energy calculations are in good agreement with the experimental values. The calculations demonstrate the preferential layer-like occupation by Cr of the interstitial sites in the compound and clearly show its metallic behaviour. In the case of the Cr_xSb_y system with the ratios $x:y = 1:2$ and $x:y = 1:3$, the calculations have been performed for different possible structures, demonstrating their physical properties expected to be observed experimentally.